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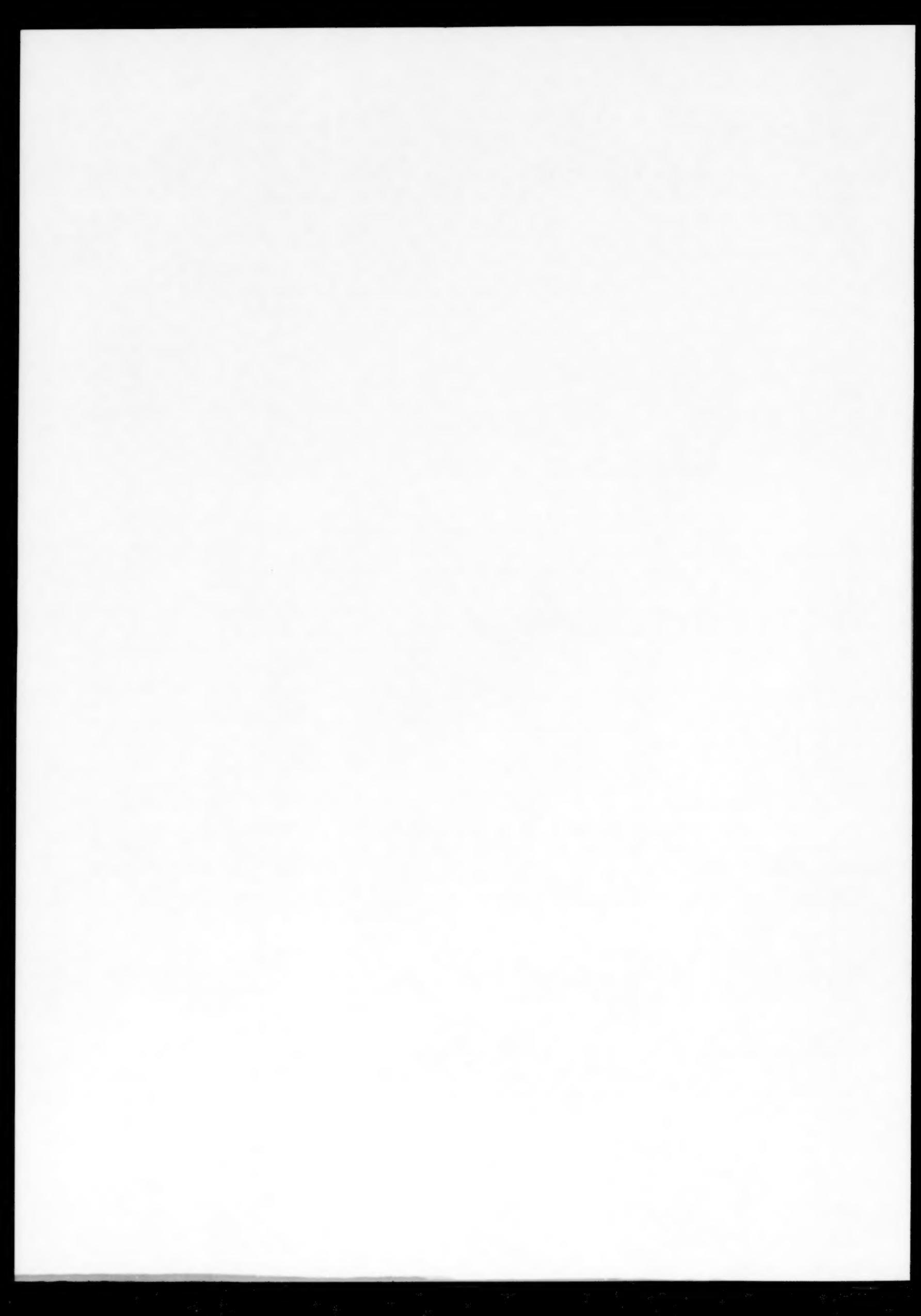
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*Ionization (incl. Rydberg states)*

The electronic states and molecular properties of 1,2,3-triazine studied by VUV absorption, near-threshold electron energy-loss spectroscopy and ab initio multi-reference configuration interaction studies, M.H. Palmer, H. McNab, I.C. Walker, M.F. Guest, M. MacDonald and M.R.F. Siggel

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